

4-Hydroxybenzoic acid  
99-96-7 | DTXSID3026647

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.09 days

Global applicability domain: Outside

Local applicability domain index: 2.82e-01

Confidence level: 8.79e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Propylbenzene</div> <div>Measured: 24.3</div> <div>Predicted: 4.02</div>	<div>Image not found</div> <div>4-Ethyltoluene</div> <div>Measured: 24.3</div> <div>Predicted: 3.95</div>	<div>Image not found</div> <div>1-Methyl-2-propylbenzene</div> <div>Measured: 12.5</div> <div>Predicted: 3.17</div>
<div>Image not found</div> <div>Ethylbenzene</div> <div>Measured: 120</div> <div>Predicted: 6.21</div>	<div>Image not found</div> <div>3-Ethyltoluene</div> <div>Measured: 12.5</div> <div>Predicted: 3.26</div>	